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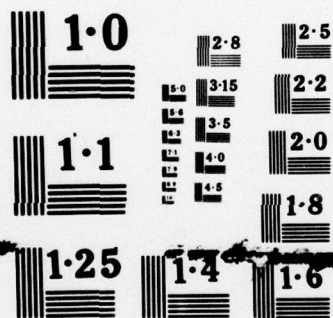
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The LEED investigations of the role of a free surface in the initiation of Marten-  
sitic phase transformations were restricted to principally cobalt surfaces and  
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## 20. ABSTRACT CONTINUED

unapplicable to the cobalt system. Detailed low-energy electron-diffraction (LEED) work on the (0001) surface of cobalt has indicated no existence of surface localized different phases or embryos that could act as nuclei for the martensitic transformation. The atomic structure of the cobalt surface was shown to be equivalent to that of the bulk in both the high temperature and low temperature phases. The soft-mode idea could therefore be examined by LEED in detail as a viable mechanism for martensitic transformation nucleation at the surface of cobalt and other transforming materials.

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FINAL TECHNICAL REPORT

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for

Research Grant No. DAAG29-77-G-0162  
"Investigation of the Initiation of Solid State Structural  
Phase Transformations at Crystal Surfaces by Low-Energy  
Electron-Diffraction (LEED)"

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The LEED investigations of the role of a free surface in the initiation of Martensitic phase transformations were restricted in the work under the Grant to principally cobalt surfaces and iron and titanium surfaces.

Our aim was to study the possible occurrence of surface localized soft phonon modes active in nucleation, however, it was first determined by LEED studies of both pre and post transformed cobalt that the traditional operational nucleation mechanism localized to a surface (surface localized "frozen in" embryos or nuclei) and proposed faulting mechanisms were unapplicable to the cobalt system. Our detailed low-energy electron-diffraction (LEED) work on the (0001) surface of cobalt has indicated no existence of surface localized different phases or embryos that could act as nuclei for the martensitic transformation. The atomic structure of the cobalt surface was shown to be equivalent to that of the bulk in both the high temperature and low temperature phases. The soft-mode idea could therefore be examined by LEED in detail as a viable mechanism for martensitic transformation nucleation at the surface of cobalt and other transforming materials.

Our LEED investigation of the (0001) cobalt surface (the habit plane in the transformation) determined initially that the single crystal sample could be cycled a large number of times (more than 20 times) through the transformation without detrimental effects to the single-crystallinity of the surface of the sample if heating and cooling rates were greater than about  $100^{\circ}\text{C}/\text{sec.}$ , i.e. that the transformation dynamics could be monitored by LEED - a technique requiring single crystal samples. Cycling showed surface transformation hysteresis effects similar to that observed in the bulk and a spread of surface transformation temperatures varying from sample-to-sample ( $450^{\circ} \pm 15^{\circ}\text{C}$ ). Most important though, LEED intensity/temperature measurements gave no indication of active surface soft-modes under the temperature cycling conditions noted.



It should be noted that the soft modes expected to be active in cobalt are transverse propagating in the  $[0001]$  direction with  $[0100]$  polarization. The surface Debye-Waller factor in the kinematic form depends on the projection of the atomic mean-square vibrational amplitude (the polarization direction) on the electron scattering vector. Therefore, LEED observations on the  $(0001)$  face of cobalt should only detect possible soft-modes for non-specular diffracted beams at small scattering angles (low energy). The monitoring of the  $(1\bar{1})$  beam at 108 eV under slow heating and cooling conditions did in fact yield indications of a possible surface soft-mode (Figure 1). The problem with the measurement was, however, that it was not repeatable due to severe degradation of the sample single-crystallinity under the slow heating and cooling rates (less than  $10^\circ\text{C}/\text{sec.}$ ). Similar measurements on a subsequent  $(0001)$  sample gave similar results: some possible softening, but loss of single-crystallinity. The statistics for the measurements are poor enough that at this point no strong claims can be made for the existence of surface soft-modes in cobalt, although the limited evidence is promising.

Additional work on the  $(10\bar{1}0)$  face of cobalt was undertaken to corroborate the existence of the alleged soft-modes. The mode propagation direction is in the plane of this surface and the polarization direction is out of the plane of this surface. Strong coupling should therefore exist between the modes anomalously high vibration amplitudes and the electron scattering vector (usually near perpendicular to the surface) and enhance observation of the mode. It was found however, that the transformation on the  $(10\bar{1}0)$  plane was not well behaved in that the single crystallinity was ruined independent of heating/cooling rates. This is probably because the hcp  $(10\bar{1}0)$  does not transform to a well behaved plane in the fcc phase (unlike  $(0001)$  hcp  $\rightarrow$   $(111)$  fcc) but to a high index stepped surface.

Further work in search of surface soft-modes was carried out on the iron (110) and (100) surface. LEED results from iron could not be obtained at or near the transformation temperature ( $\sim 910^{\circ}\text{C}$ ) because the thermal phonon scattering of electrons at such high temperature is so intense that it over-shadows the diffracted electron scattering, i.e. the coherent scattering (along with any indication of soft-mode behavior) is buried in a very high back-ground of incoherent scattering. Kinematic scattering analysis indicates that coherent scattering within a  $1/2^{\circ}$  solid angle subtended from the sample, i.e. approximately the size of a diffracted beam, should equal incoherent background scattering (multi-phonon scattering) within the same solid angle at approximately  $1000^{\circ}\text{C}$ . However, our measurements on Co, Fe and scant measurement on Ti indicate that in actually the equivalence occurs at approximately  $600^{\circ}\text{C}$  with only slight variation due to the different bulk Debye temperatures.

The above discussion has pointed out our attempts to understand the nucleation of Martensitic transformations. The principal conclusion to be currently made on our work is that there is significant information pointing to a prominent role of free surfaces in the nucleation of Martensitic transformations through surface localized soft-mode behavior. More detailed studies into such possibilities are, however, required to convincingly note the importance of free surfaces in such transformations.



Publications and Reports under the Grant:

1. "Surface Contraction of the Clean W(001) Face," B. W. Lee, A. Ignatiev, S. Y. Tong and V. A. Van Hove, J. Vac. Sci Technol 14, 291 (1977).
2. "The State of the Surface of Martensitically Transforming Cobalt Single Crystals," R. Alsenz, B. W. Lee, A. Ignatiev and M. A. Van Hove, Sol. State Comm. (1977).
3. "Surface Structures of the Two Allotropic Phases of Cobalt," B. W. Lee, R. Alsenz, A. Ignatiev and M. A. Van Hove, Phys. Rev. B (1978).
4. "LEED Observations of the State of the Surface of Martensitically Transforming Cobalt," A. Ignatiev, R. Alsenz, B. W. Lee and M. A. Van Hove, Proc. 3rd Intern. Conf. Solid Surfaces (Vienna, 1977).
5. "The Surface Structure of Epitaxially Grown Cobalt Oxide Films," A. Ignatiev, B. S. Lee and M. A. Van Hove, Proc. 3rd Intern. Conf. Solid Surfaces (Vienna, 1977).

Theses Awarded:

R. Alsenz, "Martensitic Transformation at the Surface of Cobalt," M.S. University of Houston, August 1977.

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